Development and Validation of a Predictive Model to Assess the Impact of Coastal Zone Emissions on Urban Scale Air Quality

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- Background
 - Rationale and goal of SERDP study
 - □ Local and regional impact
- Limitations of current models
 - Land-sea interface
- Model Components
 - □ MM5
 - □ LAP Model
 - Chemistry Model
 - Linkage Model
- Model Validation
- Application
- Summary



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Why did we perform this study?

- Study was funded by SERDP.
- DoD operations are sources of atmospheric pollutants and their precursors.
- Many DoD operations are located adjacent to areas that suffer from elevated levels of urban and regional scale air pollution.
- What is the impact of DoD emissions on urban scale air pollution?
- How can we reduce the DoD impact with minimal effect on DoD's mission?



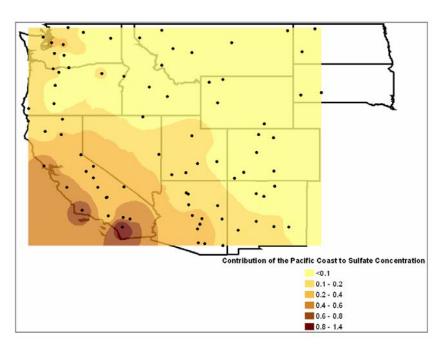
Overall Goal

Provide a tool that can be used to develop and implement effective strategies to reduce the impact of coastal operations on urban scale air quality.



Importance of Ship Emissions

- Significant source of SO₂, NO_x, and PM
- Local and regional impact



Contributions of the Pacific Coast area to the ammonium sulfate (ug/m³) in the Class I areas of the western United States based on trajectory regression

Xu et al. (2006), *Atmos. Environ*., submitted.

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Limitations of Current Model Capabilities

Meteorology

- Difficult to faithfully simulate the meteorology at the air-sea and land-sea interfaces.
- Improved forecast models and advection/dispersion models have been developed.

Air Quality

- Difficulty in determining the specific impact of emissions from individual sources on secondary air pollutants.
- There are a number of approaches that can be applied.

Emissions

- □ Large uncertainty. Updated emission factor estimates for ships, aircraft and vehicles are available.
- Activity based and fuel based emission factors can be applied.

Approach

Dispersion Air Quality No Chemical Interaction By Grid Averaging Chemical Interaction Explicitly Included Explicitly Included

- Better accounting of mean and turbulent air motions during pollutant transport.
- Chemical reactions between pollutants in different air parcels included without losing source identity.
- Hybrid model allows the determination of the contribution of each source to <u>secondary</u> pollutant formation at all receptors.



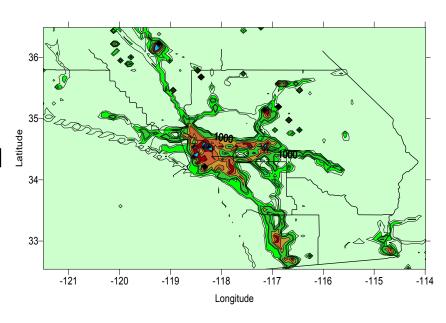
Tasks

- Task 1: Emission Inventory Development
- Task 2: Model Development
- Task 3: Model Validation
- Task 4: Reporting



- CARB 2000 annual emissions inventory
- Southern California Ozone Study 1997 (SCOS97)
 - □ 5 x 5 km gridded hourly emissions
 - Speciated organics
 - Includes commercial, civil, and military aviation sources and marine sources
- 2001 Barrio Logan Study
 - Microscale scale emissions inventory
 - Additional information on the spatial and temporal distribution of emissions

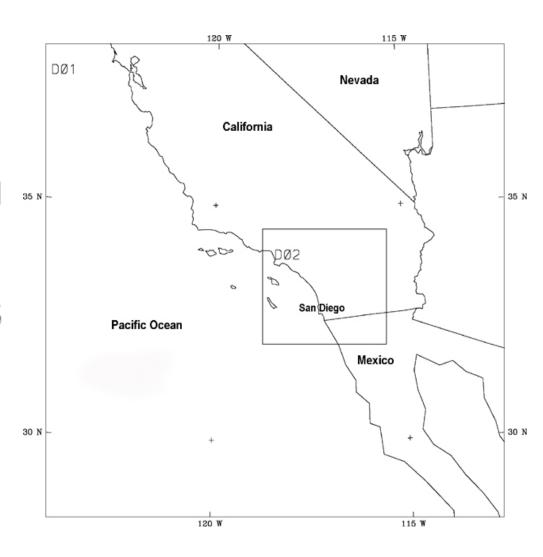
San Diego:
Daily NOx Emissions



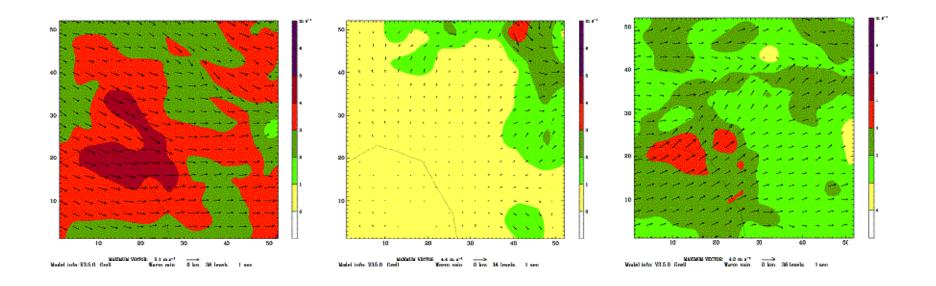


MM5

- Domains:
 - □ coarser domain grid cell size is 15 km, 75x75 cells.
 - □ inner grid cell size 5 km, 55x61 cells
- 35 layers.

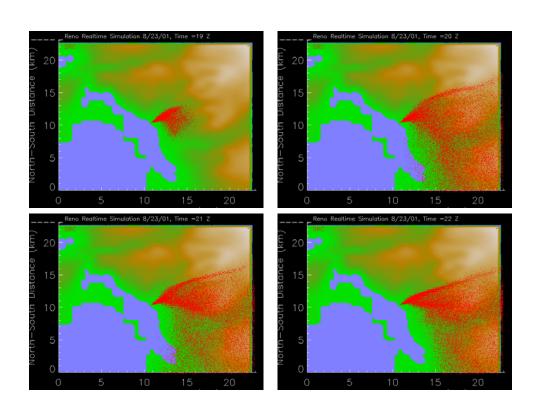


MM5 (cont.)



- •Receiving real-time MM5 output of simulated surface wind vectors and color filled wind speed vectors from NPS to drive the LPM.
- •Can also apply multiple nested grids 12, 4, 1.333, and 0.433 km to evaluate synoptic, regional scale, mesoscale, and microscale effects.

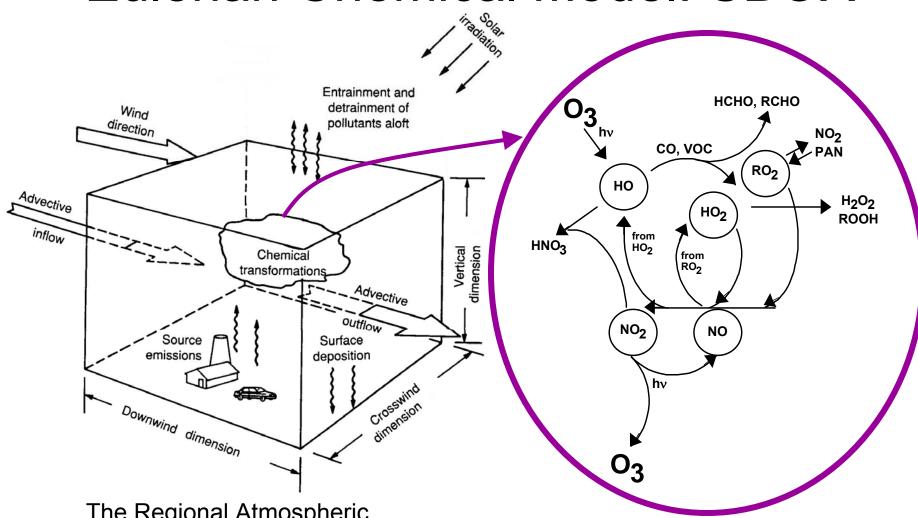
Lagrangian Particle Model



Example of a simulated tracer plume in San Diego Harbor (1-hr time intervals, noon to 4 PM).

- Incorporates wind field forecasts from MM5.
- Developed a converter that allows for a grid as fine as 0.4 km.
- Model incorporates moving and tilted emissions.

Eulerian Chemical Model: SBOX



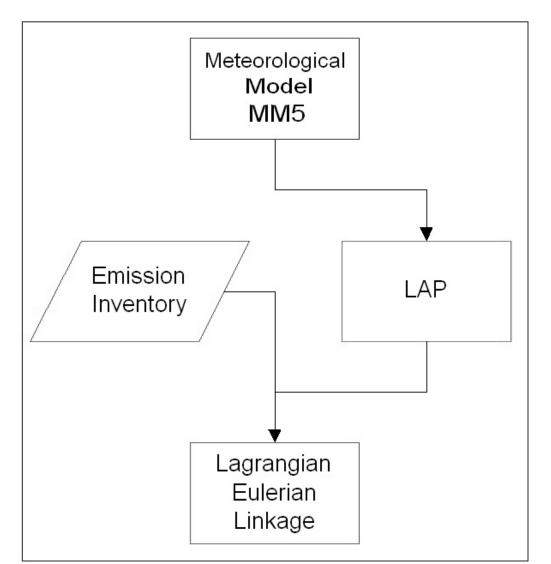
The Regional Atmospheric Chemistry Mechanism, RACM, [Stockwell et al., 1997] was used.

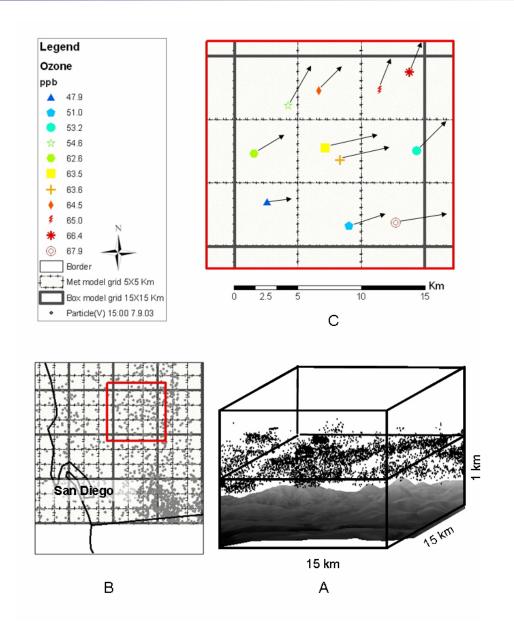
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SBOX Details

- The Regional Atmospheric Chemistry Mechanism, RACM, (Stockwell et al., 1997) was used.
 - □ RACM is a highly revised version of the RADM2 mechanism (Stockwell et al., 1990)
 - □ Includes reactions for 17 stable inorganic species and 4 inorganic intermediates. Organic species are aggregated according to their chemical structure and reactivity into 32 stable organic species and 24 organic intermediates. There are a total of 237 reactions in the RACM mechanism.
- Photolysis rate coefficients for the 23 photochemical reactions in the RACM mechanism were calculated according to Madronich (1987) with an actinic flux computed by a radiative transfer model that is based on the delta-Eddington technique (Joseph and Wiscombe, 1976).

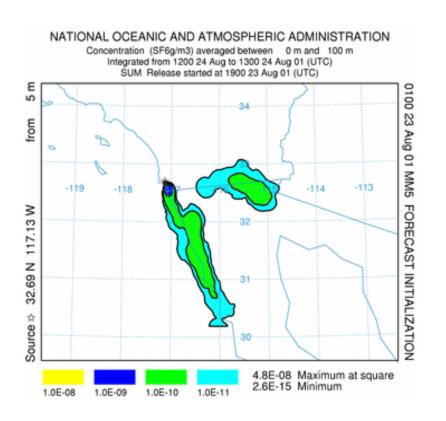


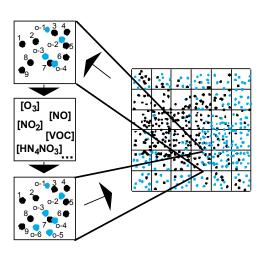




 $Particle_k(x,y,z,T,RH,p,chm_i....chm_j,ID,t)$

Additional Model Development





Worked collaboratively with NOAA:

- •Evaluated of HYSPLT-Chem model performance.
- •Compared predictions from the DRI and NOAA models.

Additional Model Development (cont.)

LPM Testing:

- Obtained CARB tracer data from the 2001 Barrio Logan Study.
- Evaluated LPM predictions



Model Validation



- 10 Research flights performed in July 2003 during mid-day (1200-1700), sampling a grid of ~100x80 km
- Measurements included:
 - □ Trace gases (CO, SO₂, NO, NO₂, NO_y, O₃ and NO₃-)
 - \square Aerosol (3 λ nephelometer)
 - Meteorological parameters (WS, WDD, T, RH and P)
 - □ Location (GPS)
 - Grab samples for HC and carbonyl analysis

On-Board TVA's Research Aircraft



Airborne Data System



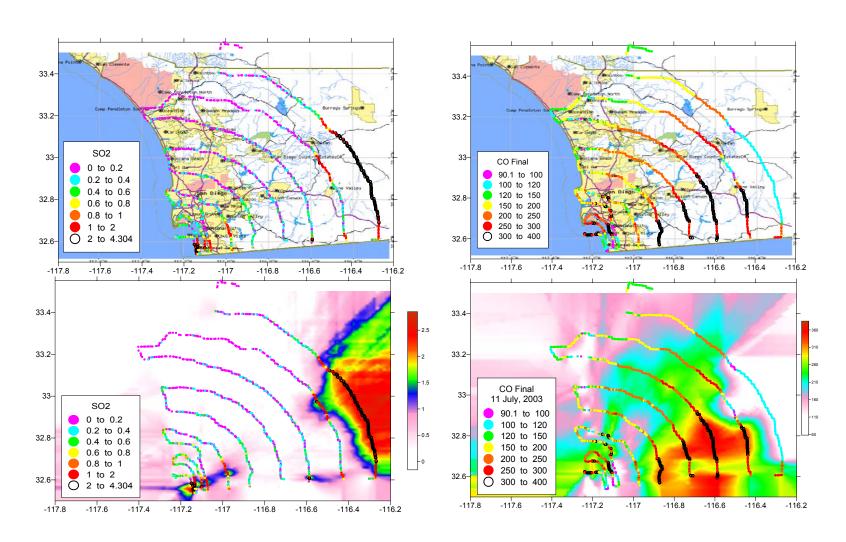


Segment	
1	Altitude profile over the airport up to 6000'
2	Level flight at 6000' to a way point east of the SD harbor
3	Altitude profile over the mid-way point down to 1000'
4	Constant elevation sampling at ~1000' over the surface for 4-5 h
5	Once an hour zero calibration for approx. 5 min
6	Ascend to 6000' and fly toward the airport
7	Altitude profile over the airport from 6000' to the surface
8	Multipoint calibration of All gas analyzers

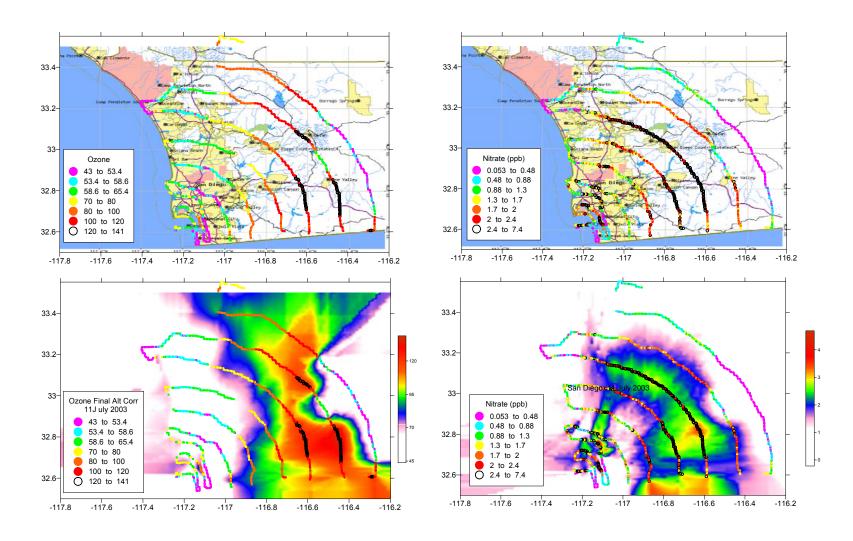




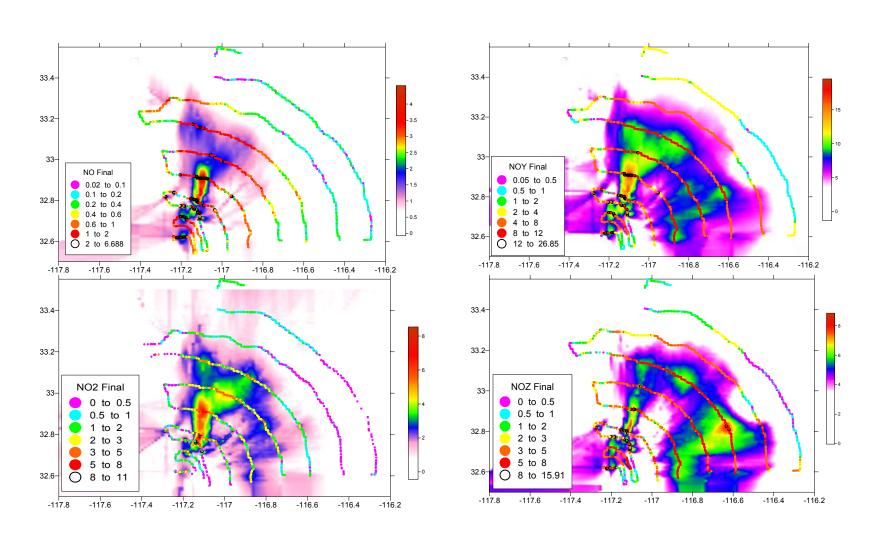
SO₂ and CO



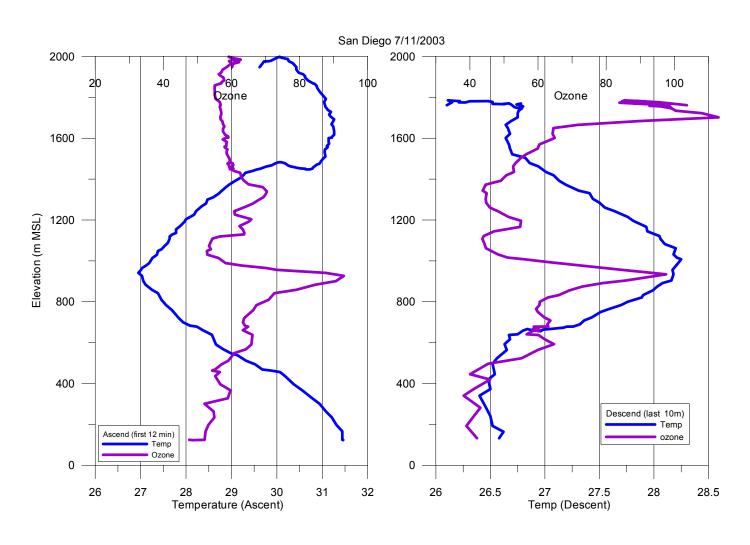
O₃ and Nitrate



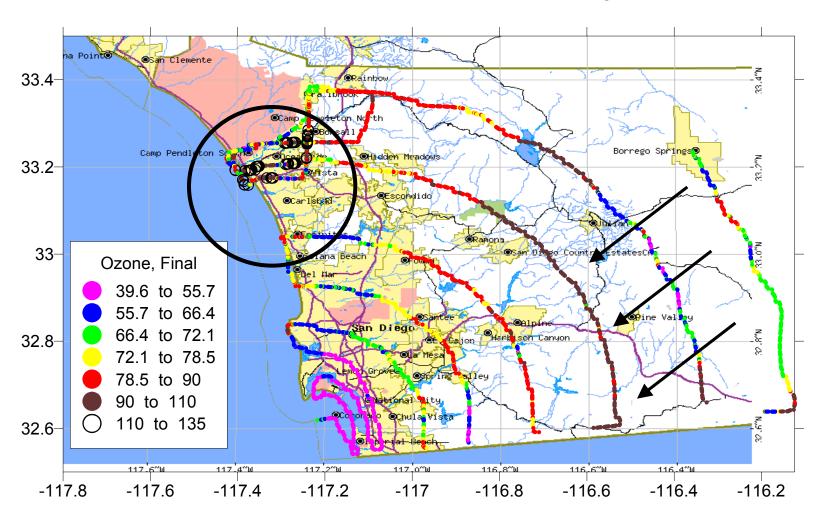
Conversion of NO to NO_z



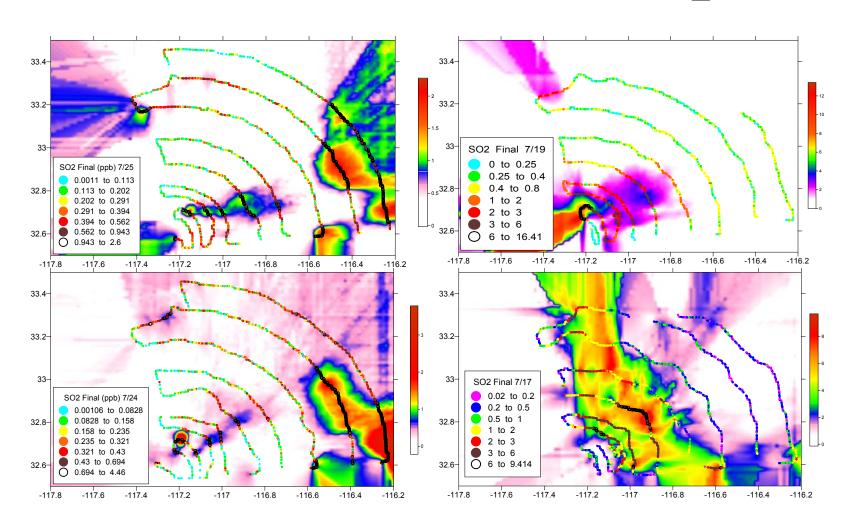
O₃ and Temperature Profiles



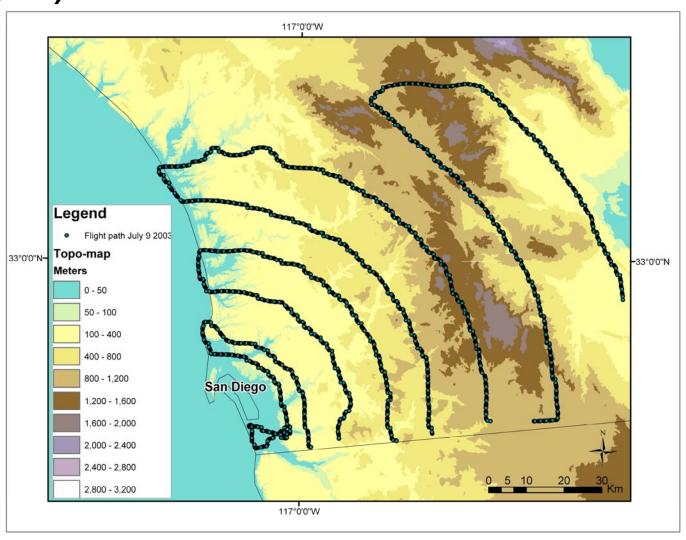
Ozone Transport from the North and Local Ozone 13 July 2003



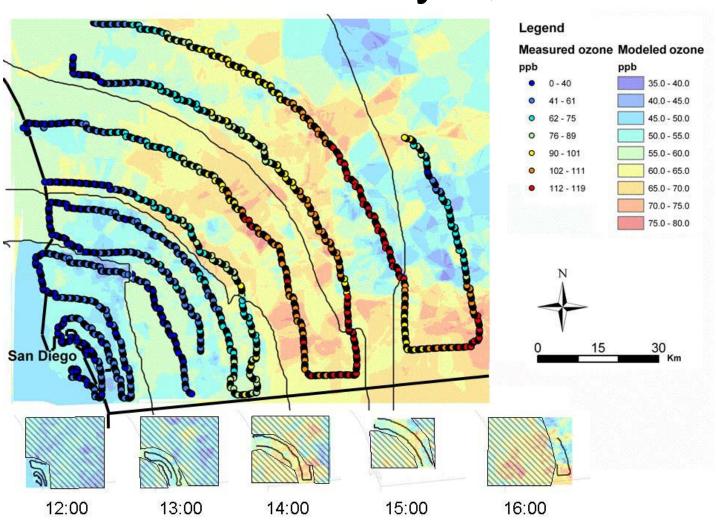
Local and Transported SO₂



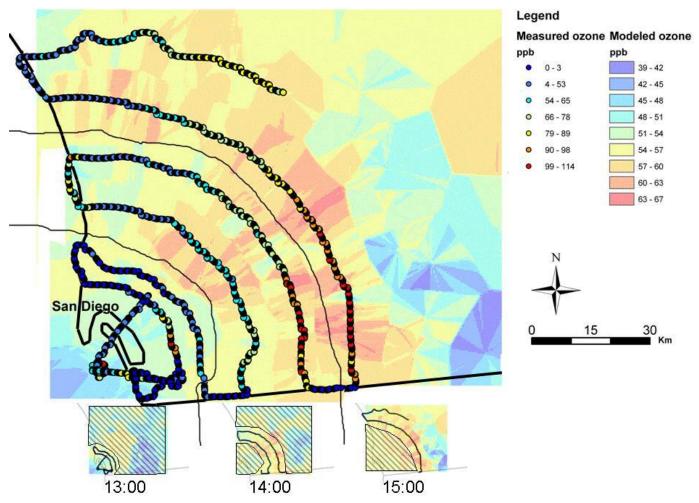
Model Results: Map of study (flight) area



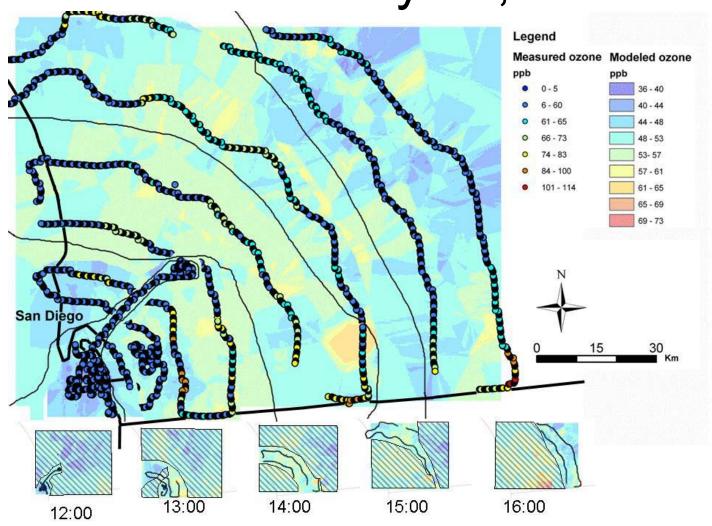
Model Results vs. Airborne Measurements: July 7, 2003



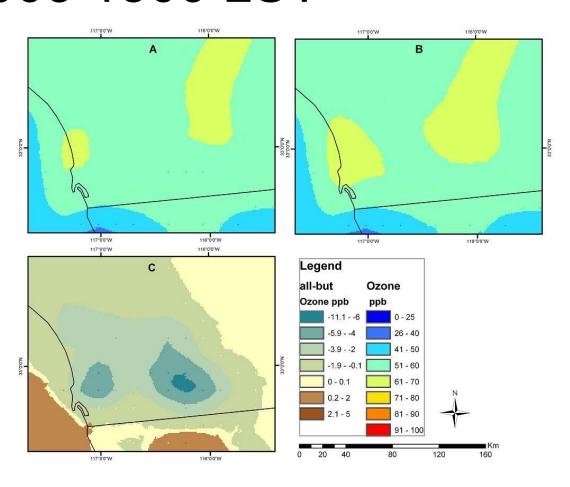
Model Results vs. Airborne Measurements: July 9, 2003



Model Results vs. Airborne Measurements: July 17, 2003

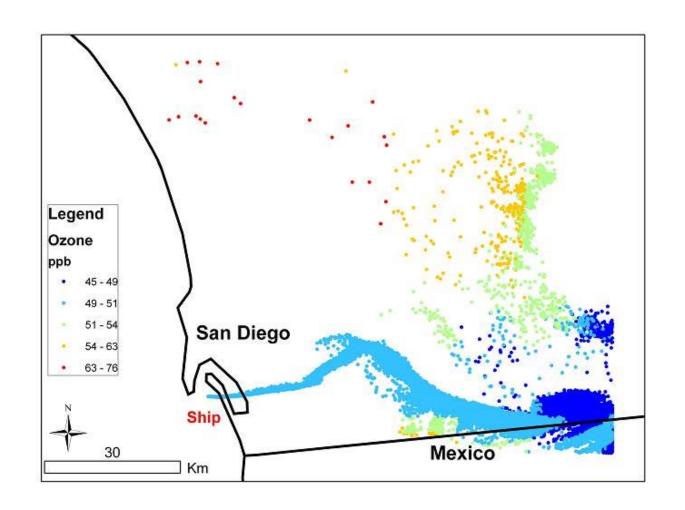


Ozone concentration (ppb), July 19 2003 1500 LST



A: All sources, B: Without DoD emissions, C: Difference

Example of impact of emissions form a single ship in San Diego harbor at July 7 2003 1500 LST



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Summary

- Developed and validated a hybrid model to assess the impact of coastal emissions on air quality.
- Incorporates the strengths of both the Lagrangian transport/diffusion model and Eulerian multi box chemical model.
- Capable of evaluating impact of emissions from individual sources (i.e. source/receptor relationship).
- Modeling system is modular and can incorporate different transport/diffusion and transformation schemes.
- System can evaluate moving sources such as ship and aircraft emissions.
- Employed comprehensive platform for measuring emissions from individual sources and pollutant transport and transformation.
- Unique database for future model evaluation studies.

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